Design of enantioselective catalysts in MOF architectures: a combined theoretical and experimental approach

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In the last decades salen complexes have proven their value as chiral epoxidation catalysts[1]. The original manganese-salen complex allows the enantioselective epoxidation of unfunctionalized olefins with an enantiomeric excess of over 90%[2]. To improve the applicability of this catalyst, a heterogenization method is proposed where the homogeneous catalyst is trapped inside the cages of a nanoporous material. As carrier material NH_2-MIL101(Al)[3] is chosen. This metal organic framework (MOF) is known for its high internal surface area and large cavities. The encapsulation is done via a one pot synthesis where the complex is added to the mixture during MOF synthesis.

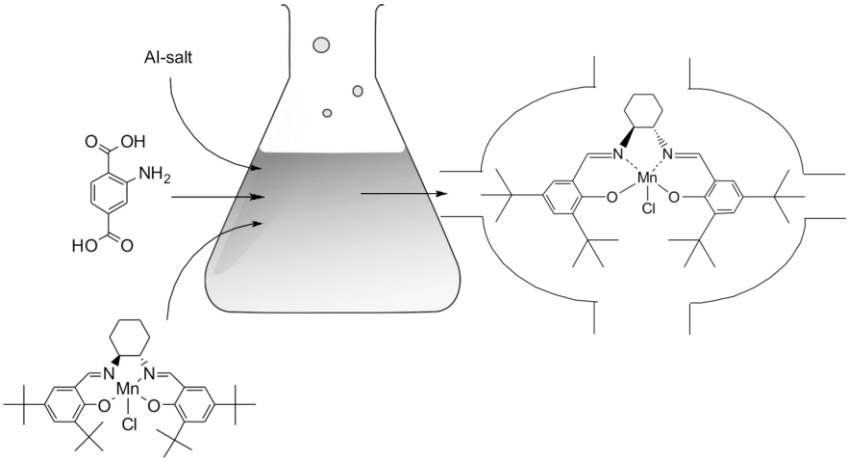

Figure 1: Principle of the one pot synthesis

Molecular modeling techniques were used to analyze the various spectroscopic results, indicating the successful immobilization of the complex. Similar techniques were also employed to investigate the reaction mechanism of this epoxidation, especially the influence of the spin state on the manganese center. Eventually the host influence on the activity can also be unraveled. With this combination of experiments and theory a heterogeneous catalyst that offers similar selectivity as the homogeneous counterpart is designed.

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[3] Hartmann, M.; Fischer, M., *Microporous Mesoporous Mat.*, (2012) **164**, 38.